

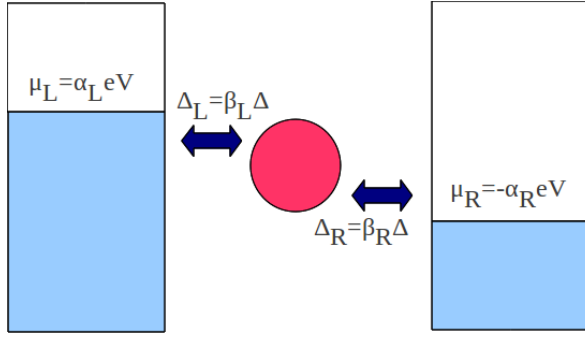
# Nonequilibrium conductance of a nanodevice for small bias voltage

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**Abstract.** Using non-equilibrium renormalized perturbation theory, we calculate the retarded and lesser self energies, the spectral density  $\rho(\omega)$  near the Fermi energy, and the conductance  $G$  through a quantum dot as a function of a small bias voltage  $V$ , in the general case of electron-hole asymmetry and intermediate valence. The linear terms in  $\omega$  and  $V$  are given exactly in terms of thermodynamic quantities. When the energy necessary to add the first electron ( $E_d$ ) and the second one ( $E_d + U$ ) in the quantum dot are not symmetrically placed around the Fermi level,  $G$  has a linear term in  $V$  if in addition either the voltage drop or the coupling to the leads is not symmetric. The effects of temperature are discussed. The results simplify for a symmetric voltage drop, a situation usual in experiment.

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**Figure 1.** (Color online) Scheme of the system. A QD (circle) is connected to the left ( $L$ ) and right ( $R$ ) conducting leads, with a difference  $eV$  between the corresponding chemical potentials. Each lead hybridizes with the dot level providing a contribution  $\beta_\nu \Delta$  to the resonant width  $\Delta$ .

## 1. Introduction

Recently, there has been great interest in the conductance through one quantum dot (QD) for low applied bias voltage and temperature, searching for universal scaling properties [1, 2, 3, 4, 5, 6, 7]. In experiments [1, 2, 7, 8] a semiconductor QD or a single molecule is attached to two conducting leads (left  $L$  and right  $R$ ), a bias voltage  $V$  is applied between the leads (see Fig. 1), and the conductance  $G = dI/dV$ , where  $I$  is the current, is measured. For  $V = 0$ , the temperature dependence of the conductance has been found to be very well described by the same universal function  $G(T/T_K)$ , where  $T_K$  is the Kondo temperature, even for systems with very different  $T_K$  [1, 8]. This scaling law had been obtained from numerical renormalization group (NRG) calculations of the impurity Anderson model [9] in the Kondo regime ( $-E_d \gg \Delta$  and  $E_d + U \gg \Delta$ , where the Fermi energy is set as 0,  $E_d$  is the on-site energy,  $U$  the Coulomb repulsion and  $\Delta$  the resonant level width).

In the non equilibrium situation  $V \neq 0$ , the problem is much tougher theoretically. In this situation, exact Bethe ansatz results are available only for a simpler problem (the interacting resonance level model) [10] while NRG methods have serious limitations [11]. In some works, the spectral density  $\rho_\sigma(\omega)$  calculated with NRG at equilibrium is used to calculate non-equilibrium properties, assuming that  $\rho_\sigma(\omega)$  is not affected very much by an applied bias voltage  $V$  [12, 13, 14, 15]. However, this approach misses the effects of broadening of  $\rho_\sigma(\omega)$  caused by  $V$ , and as a consequence, the results are quantitatively and in some cases even qualitatively different than the correct ones [16].

In the Kondo limit, for either  $eV \gg kT_K$ , or  $\mu_B B \gg kT_K$  in presence of an applied magnetic field  $B$ , have been determined using perturbation theory and poor man's scaling [17]. Using a Fermi liquid approach, based on perturbation theory in  $U$  (PTU [18, 19, 20, 21]), and Ward identities, Oguri has determined exactly the scaling up to second order in  $kT$  and  $eV$  for the symmetric Anderson model [22, 23]. Further work considered the effect of higher order contributions using different approximations, like PTU [3], non-crossing approximation [5], or decoupling of equations of motion [6].

The effect of asymmetric coupling to the leads  $\Delta_L \neq \Delta_R$  [defined by Eq. (3)], and asymmetric drop in the bias voltage [ $\alpha_L \neq \alpha_R$ , see Eq. (2)] has been calculated up to second order in  $T$  and  $V$  using Fermi liquid approaches, for the symmetric Anderson model ( $-E_d = E_d + U$ ) [3, 4]. In other works electron-hole asymmetry was present for  $V = 0$  but symmetric voltage drop and coupling to the leads was assumed [5, 6]. In all these works, the linear terms in  $T$  and  $V$  are absent, and the conductance is maximum for  $T = V = 0$ . In this work, we calculate exactly the linear term in  $V$  in terms of thermodynamic quantities at equilibrium. This term is non vanishing if  $-E_d \neq E_d + U$  and in addition either  $\Delta_L \neq \Delta_R$  or  $\alpha_L \neq \alpha_R$ . Previous work for the infinite  $U$  Anderson model, a  $1/N$  expansion [24] predicts that the conductance has a linear term in  $V$  of the form  $2(\Delta_R - \Delta_L)eV/(\Delta kT_K)$  for  $\alpha_L = \alpha_R$ .

A comparison of recent theoretical studies of the scaling properties [3, 4, 5] with experiment indicates that some degree of intermediate valence (a deviation from the Kondo regime) is necessary to explain the experimental data of Grobis *et al.* [1], in which the effect of  $V$  to decrease the conductance is about 2/3 smaller than that expected in the Kondo regime. A good agreement with this experiment is obtained using the Anderson model [3, 5], while the experimental results of Scott *et al.*, [2] seem to be out of the reach of the model (see Section 4). For semiconductor QD's, it is believed that the Coulomb repulsion  $U$  is not too large in comparison with the resonant level width  $\Delta = \Delta_R + \Delta_L$  [25]. In a recent experiment in which the shot noise is measured, these parameters were estimated as  $U = 0.56$  and  $\Delta = 0.17$  meV respectively [26].

The above facts suggest that the expansion parameter in PTU  $U/\pi\Delta$  is of order one, and then PTU might be a useful approach. In fact, PTU up to second order in  $U$  (using an interpolative scheme to recover the atomic limit [27, 28]) has been shown to describe well the equilibrium conductance for  $U/\pi\Delta \lesssim 2$  [29]. The results agree with those obtained using the finite temperature density matrix renormalization group method [30]. Interpolative PTU has also been used to calculate persistent currents in rings with an embedded QD or side coupled to a QD [31], giving results in agreement with exact calculations in small systems [31], and renormalization group results [32] for  $U = 6.25\Delta$ . Other applications at equilibrium include impurities in quantum corrals [33, 34], magnetoconductance [35], and conductance through Hubbard chains [36].

The extension of PTU up to second order to the non equilibrium (finite  $V$ ) case has been first considered by Hershfield *et al.*, [37]. They found that for finite  $V$ , the current is conserved only in the electron-hole symmetric Anderson model. Different self-consistent approaches were proposed to overcome this shortcoming, by a suitable election of the unperturbed Hamiltonian [27, 38]. While these approaches work well in absence of a magnetic field  $B$ , numerical difficulties were found for small non-vanishing  $B$  and  $V$  [38]. Applications of PTU up to forth order (which seem necessary to obtain a splitting of the spectral density for large enough  $V$ ) [39, 40], or calculations of the noise spectrum [41, 42] were restricted to the symmetric model. We show in this work that the current is conserved up to terms of order  $V^3$  without the need of adjusting the unperturbed Hamiltonian. We use renormalized PTU (RPTU) to calculate the conductance for low

V. The basic idea of RPTU as developed by Hewson [43] is to reorganize the PTU in terms of fully dressed quasiparticles in a Fermi liquid picture. The parameters of the original model are renormalized and their values can be calculated exactly from Bethe ansatz results [44, 45, 46, 47, 48], or accurately using NRG [49, 50, 51, 52, 53]. One of the main advantages is that the renormalized expansion parameter  $\tilde{U}/(\pi\tilde{\Delta}) \ll 1$ , being 1 in the extreme Kondo regime ( $U \rightarrow \infty$ ). Here we assume  $B = 0$ . Exact results for small magnetic field were obtained using RPTU in the symmetric case [52], while for large  $B$ , calculations with interpolative PTU were presented [38].

We calculate the self energies and the spectral density near the Fermi energy for small values of the frequency  $\omega$  and bias voltage  $V$ , and the conductance for small  $V$ . The linear terms in  $\omega$  and  $V$  are given exactly in terms of the occupation at the dot, magnetic susceptibility and specific heat at equilibrium. The lesser self energy is given exactly up to quadratic terms. We also show that the current is conserved up to terms of order  $V^3$  in PTU.

The paper is organized as follows. In Section II we describe the system and the impurity Anderson model used to represent it. We also review briefly the formalism of the perturbation theory and the idea of RPTU. Section III contains the results of the calculations, and several limiting cases of interest in which the general expressions become simpler. Section 4 contains a summary and a discussion.

## 2. Model and formalism

### 2.1. Model

A scheme of the model is displayed in Fig. 1. The QD interacting with two conducting leads is described by the spin 1/2 Anderson model. In general, to use PTU, it is convenient to split the Hamiltonian into a noninteracting part  $H_0$  and a perturbation  $H'$  as

$$\begin{aligned} H &= H_0 + H', \\ H_0 &= \sum_{k\nu\sigma} \varepsilon_{k\nu} c_{k\nu\sigma}^\dagger c_{k\nu\sigma} + \sum_{\sigma} \varepsilon_{eff}^{\sigma} n_{d\sigma} \\ &\quad + \sum_{k\nu\sigma} \left( V_{k\nu} c_{k\nu\sigma}^\dagger d_{\sigma} + \text{H.c.} \right), \\ H' &= \sum_{\sigma} (E_d - \varepsilon_{eff}^{\sigma}) n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}, \end{aligned} \tag{1}$$

where  $n_{d\sigma} = d_{\sigma}^\dagger d_{\sigma}$ , and  $\nu = L, R$  refers to the left and right leads, with chemical potentials

$$\mu_L = \alpha_L eV, \quad \mu_R = -\alpha_R eV. \tag{2}$$

respectively, with  $\alpha_L + \alpha_R = 1$ . Similarly, the couplings to the leads assumed independent of frequency are expressed in terms of the total resonant level width

$\Delta = \Delta_L + \Delta_R$  as

$$\Delta_\nu = \pi \sum_k |V_{k\nu}|^2 \delta(\omega - \varepsilon_{k\nu}) = \beta_\nu \Delta. \quad (3)$$

In general  $\varepsilon_{eff}^\sigma$  is determined selfconsistently, except for the electron-hole symmetric case with  $B = 0$ , for which  $\varepsilon_{eff}^\sigma = 0$  [27, 38].

## 2.2. Green's functions and self energies

The one-particle properties of the system, including the current, are determined by three types of independent one-particle Green's functions, the retarded  $G^r(\omega)$ , the advanced  $G^a(\omega)$  which are the complex conjugate of  $G^r(\omega)$ , and the lesser ones  $G^<(\omega)$ . The retarded Green's function of the electrons at the dot for spin  $\sigma$ , can be written as

$$G_{d\sigma}^r(\omega) = \frac{1}{\omega - \varepsilon_{eff}^\sigma + i\Delta - \Sigma_\sigma^r(\omega)}. \quad (4)$$

In PTU up to second order in  $U$ , the retarded self energy is approximated as [38]

$$\Sigma_\sigma^r(\omega) = E_d^\sigma - \varepsilon_{eff}^\sigma + U \langle n_{d\bar{\sigma}} \rangle + \Sigma_\sigma^{r2}(\omega), \quad (5)$$

where  $\Sigma_\sigma^{r2}$  contains the contribution of order  $U^2$ .

The lesser Green's function can be written in the form [38]

$$G_{d\sigma}^<(\omega) = |G_{d\sigma}^r(\omega)|^2 \left( \frac{g_{d\sigma}^<(\omega)}{|g_{d\sigma}^r(\omega)|^2} - \Sigma_\sigma^<(\omega) \right), \quad (6)$$

where  $g_{d\sigma}^r(\omega)$ ,  $g_{d\sigma}^<(\omega)$  are the retarded and lesser noninteracting Green's functions, and  $\Sigma_\sigma^<(\omega)$  is the lesser self energy.

For large values of  $U/\Delta$ , ordinary PTU in  $U$  is not reliable and Hewson proposed to reorganize the perturbation series in terms of renormalized parameters (which we denote with a tilde) such that  $\tilde{U}/(\pi\tilde{\Delta}) \leq 1$ . Within RPTU, the low frequency part of  $G_{d\sigma}^r(\omega)$  is approximated as [43]

$$G_{d\sigma}^r(\omega) \simeq \frac{z}{\omega - \tilde{\varepsilon}_{eff}^\sigma + i\tilde{\Delta} - \tilde{\Sigma}_\sigma^r(\omega)}, \quad (7)$$

where

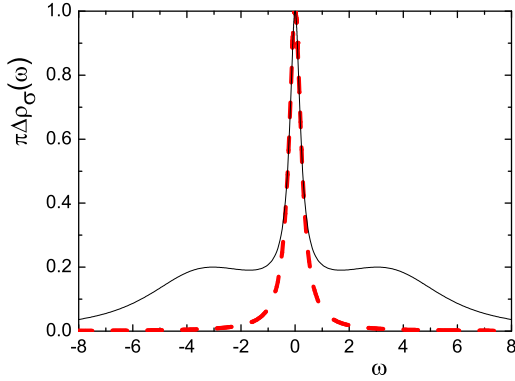
$$\begin{aligned} z &= [1 - \partial \Sigma_\sigma^r / \partial \omega]^{-1}, \quad \tilde{\varepsilon}_{eff}^\sigma = z[\varepsilon_{eff}^\sigma + \Sigma_\sigma^r(0)], \\ \tilde{\Delta} &= z\Delta, \quad \tilde{\Sigma}_\sigma^r(\omega) = z\Sigma_\sigma^{\text{rem}}(\omega), \end{aligned} \quad (8)$$

and the remainder retarded self-energy is defined as

$$\Sigma_\sigma^{\text{rem}}(\omega) = \Sigma_\sigma^r(\omega) - \Sigma_\sigma^r(0) - \omega \partial \Sigma_\sigma^r / \partial \omega. \quad (9)$$

In Eqs. (7) and (9),  $\Sigma_\sigma^r(0)$  and  $\partial \Sigma_\sigma^r / \partial \omega$  are evaluated at  $\omega = T = V = 0$ .

In Fig. 2 we compare the spectral density  $\rho_\sigma(\omega) = -\text{Im}G_{d\sigma}^r(\omega)/\pi$  evaluated within PTU up to second order with the corresponding noninteracting renormalized result



**Figure 2.** (Color online) Full line: spectral density of the Anderson model for  $U = 7\Delta$  and  $E_d = -U/2$ . Dashed line: corresponding result for non-interacting quasiparticles (see text).

( $z\tilde{\rho}_0(\omega) = -\text{Im}\tilde{G}_{d\sigma}^r(\omega)/\pi$  with  $\tilde{\Sigma}_\sigma(\omega) = 0$ ) obtained from Eqs. (7) and (8) for the symmetric Anderson model ( $\tilde{\varepsilon}_{eff}^\sigma = 0$ ). We obtain  $z = 0.2744$  for the parameters of the figure. This comparison has been made by Rejec and Ramšak for other parameters [55]. One can see that already non-interacting quasiparticles reproduce rather well the low-energy behavior. A similar comparison, for a case with non-trivial frequency dependent  $\Delta(\omega)$  has also been made [56], showing also a very good agreement for low  $|\omega|$ . An accurate calculation of  $\tilde{\Sigma}_\sigma(\omega)$  including high orders in the perturbation expansion, should lead in turn to a precise description of the spectral density at high energies, since nothing is lost in the reorganization of the perturbative expansion. However, the calculation of higher order terms becomes involved due to the need of considering counterterms and corrections to the parameters [43].

The spectral density evaluated at the Fermi energy is related with the occupancy by the Friedel sum rule [54]

$$\rho_\sigma(0) = \frac{\sin^2(\pi\langle n_{d\sigma} \rangle)}{\pi\Delta}, \quad (10)$$

which allows one to relate the effective dot level with its occupancy, using Eq. (7)

$$\tilde{\varepsilon}_{eff}^\sigma = \tilde{\Delta} \cot(\pi\langle n_{d\sigma} \rangle). \quad (11)$$

$\tilde{\Sigma}_\sigma^{\text{rem}}(\omega)$  can be calculated perturbatively using a renormalized interaction  $\tilde{U}$  which is given by the vertex function  $\Gamma$  at the Fermi energy [43, 49]. In absence of magnetic field, the subscript  $\sigma$  can be dropped. The linear term in the specific heat and the impurity contribution to the magnetic susceptibility (determined using Ward identities) are given by [43]

$$\gamma_C = 2\pi^2 k \tilde{\rho}_0(0)/3, \quad (12)$$

$$\chi = (g\mu_B)^2 (1 + \tilde{U}\tilde{\rho}_0(0))/2, \quad (13)$$

where

$$\tilde{\rho}_0(\omega) = \frac{\tilde{\Delta}/\pi}{(\omega - \tilde{\varepsilon}_{eff})^2 + \tilde{\Delta}^2} \quad (14)$$

is the density of free renormalized quasiparticles. Eqs. (10), (12), (13) and an accurate knowledge of thermodynamic quantities from Bethe ansatz or NRG, permits a precise determination of  $z = \rho(0)/\tilde{\rho}_0(0)$ , and the renormalized interaction through the Wilson ratio  $R = 1 + \tilde{U}\tilde{\rho}_0(0)$ .

To order  $\tilde{U}^2$ , the renormalized self energies can be written as [38]

$$\begin{aligned} \tilde{\Sigma}^r(\omega) = \tilde{U}^2 \int d\epsilon_1 d\epsilon_2 d\epsilon_3 & \frac{\tilde{\rho}_0(\epsilon_1)\tilde{\rho}_0(\epsilon_2)\tilde{\rho}_0(\epsilon_3)}{\omega + \epsilon_3 - \epsilon_1 - \epsilon_2 + i\eta} \\ & \times [(1 - \tilde{f}(\epsilon_1))(1 - \tilde{f}(\epsilon_2))\tilde{f}(\epsilon_3) \\ & + \tilde{f}(\epsilon_1)\tilde{f}(\epsilon_2)(1 - \tilde{f}(\epsilon_3))], \end{aligned} \quad (15)$$

$$\begin{aligned} \tilde{\Sigma}^<(\omega) = z\Sigma^<(\omega) \\ = -2i\pi\tilde{U}^2 \int d\epsilon_1 d\epsilon_2 & \tilde{\rho}_0(\epsilon_1)\tilde{\rho}_0(\epsilon_2)\tilde{\rho}_0(\epsilon_1 + \epsilon_2 - \omega) \\ & \times \tilde{f}(\epsilon_1)\tilde{f}(\epsilon_2)(1 - \tilde{f}(\epsilon_1 + \epsilon_2 - \omega)), \end{aligned} \quad (16)$$

where  $\eta$  is a positive infinitesimal and  $\tilde{f}(\omega) = \sum_\nu \beta_\nu(\omega)f(\omega - \mu_\nu)$  is an average of the Fermi functions at the two leads [ $f(\omega) = 1/(e^{\omega/kT} + 1)$ ].

### 2.3. The current

Using the Keldysh formalism [57, 58], it has been shown that the current flowing between the left lead and the dot is

$$I_L = \frac{4ie\Delta_L}{h} \int d\omega [2if(\omega - \mu_L)\text{Im}G_d^r(\omega) + G_d^<(\omega)]. \quad (17)$$

Similarly, the current with spin  $\sigma$  flowing between the dot and the right lead is

$$I_R = -\frac{4ie\Delta_R}{h} \int d\omega [2if(\omega - \mu_R)\text{Im}G_d^r(\omega) + G_d^<(\omega)]. \quad (18)$$

Of course, since the current is conserved one should have  $I_L = I_R = I$ . Then, from a weighted average of both expressions,  $G_d^<$  can be eliminated, giving [58]

$$I = \frac{8\pi\beta_L\beta_R e\Delta}{h} \int d\omega \rho(\omega)[f(\omega - \mu_L) - f(\omega - \mu_R)]. \quad (19)$$

### 3. Self energies, spectral density and conductance for small bias voltage

#### 3.1. Self energies

It is easy to see that to evaluate the differential conductance  $G = dI/dV$  at zero temperature to order  $V^n$ , it is enough to calculate the spectral density and self energies up to total order  $n$  in  $\omega$  and  $V$  (all terms of the form  $\omega^l V^{m-l}$ , with  $0 \leq m \leq l$ ,  $l \leq n$ ), since the effective interval of integration in Eq. (19) is  $eV$ , because the Fermi functions  $f(\omega)$  become step functions  $\theta(-\omega)$  at  $T = 0$ . For the same reason, the intervals of the two integrations in Eq. (16) are of order  $eV$ , and therefore one obtains  $\tilde{\Sigma}^<(\omega)$  up to terms of second order, taking  $\tilde{\rho}_0(\epsilon)$  at the Fermi energy  $\epsilon = 0$ . Performing the integration we find

$$\begin{aligned} \tilde{\Sigma}^<(\omega) = & -i\pi[\tilde{\rho}_0(0)]^3\tilde{U}^2 \\ & \times \{ \theta(\alpha_L eV - \omega)\beta_L(\beta_L^2 + 2\beta_R^2)(\alpha_L eV - \omega)^2 \\ & + \theta(-\alpha_R eV - \omega)\beta_R(2\beta_L^2 + \beta_R^2)(\alpha_R eV + \omega)^2 \\ & + \theta[(1 + \alpha_L)eV - \omega]\beta_L^2\beta_R[(1 + \alpha_L)eV - \omega]^2 \\ & + \theta[-(1 + \alpha_R)eV - \omega]\beta_L^2\beta_R[(1 + \alpha_R)eV + \omega]^2 \}. \end{aligned} \quad (20)$$

Using  $\text{Im}(\omega + i\eta)^{-1} = -i\pi\delta(\omega)$  and Eq. (15) it is easy to realize that the above arguments also work for  $\text{Im}\tilde{\Sigma}(\omega)$  and performing the two remaining integrations [after the use of the delta function  $\delta(\omega + \epsilon_3 - \epsilon_1 - \epsilon_2)$ ] one obtains up to terms of second order in  $\omega$  and  $V$

$$\begin{aligned} \text{Im}\tilde{\Sigma}^r(\omega) = & -\frac{\pi}{2}[\tilde{\rho}_0(0)]^3\tilde{U}^2[\omega^2 - 2\gamma\omega eV + \delta(eV)], \\ \gamma = & \alpha_L\beta_L - \alpha_R\beta_R, \\ \delta = & \gamma^2 + 3\beta_L\beta_R, \end{aligned} \quad (21)$$

as previously found by Oguri [23].

Note that higher order terms in the perturbation series in  $\tilde{U}$  would lead to terms of higher order in  $V$ . Therefore, the above results are exact. They can be used to test approximations. For example, from Eqs. (20) and (21), one realizes that the approximation for the lesser self energy  $\tilde{\Sigma}^<(\omega) \simeq 2i\tilde{f}(\omega)\text{Im}\tilde{\Sigma}^r(\omega)$  used in decoupling approximations [59, 6, 60], is only valid for  $V = 0$  (or  $U = 0$ ).

From Eqs. (6), (7), (8), (17) and (18) one obtains

$$I_L - I_R = -\frac{4e}{z\hbar} \int d\omega |G_d^r(\omega)|^2 [2\tilde{f}(\omega)\text{Im}\tilde{\Sigma}^r(\omega) + i\tilde{\Sigma}^<(\omega)]. \quad (22)$$

The integral introduces another factor  $eV$ . Thus, in order to obtain  $I_L - I_R$  to order  $V^3$ , one can replace  $|G_d^r(\omega)|^2$  by its value at  $\omega = 0$  and move it outside the integral.



Using Eqs. (20) and (21) the integral turns out to vanish. Then  $I_L - I_R = O(V^4)$  and the current is conserved up to order  $V^3$ .

In contrast to  $\tilde{\Sigma}^<(\omega)$  and  $\text{Im}\tilde{\Sigma}^r(\omega)$ , an accurate calculation of the real part of the retarded self energy is more difficult. As it is apparent from Eq. (15) or alternative expressions [37, 38], the calculation of  $\text{Re}\tilde{\Sigma}^r(\omega)$  involves an integration at high energies, for which the approximation given by noninteracting quasiparticles [Eq. (7) neglecting  $\tilde{\Sigma}^r(\omega)$ ] is not good enough (see Fig. 2). Fortunately  $\tilde{\Sigma}^r(0) = 0$  and  $\partial\tilde{\Sigma}^r(\omega)/\partial\omega = 0$  by construction [see Eqs. (8) and (9)], while  $\partial\tilde{\Sigma}^r/\partial eV$  can be calculated from Ward identities: using the results of Oguri [23], one sees that  $\partial\tilde{\Sigma}^r/\partial eV = \gamma\partial\tilde{\Sigma}^r/\partial\mu$ , where  $\mu$  is a shift of both chemical potentials. In addition, using Eqs. (3.15) to (3.18) of Ref. [19], and  $\partial\tilde{\Sigma}^r/\partial\omega = 0$ , one obtains  $\partial\tilde{\Sigma}^r/\partial\mu = \tilde{\rho}_0(0)\tilde{U}$ . Combining both results one has

$$\partial\tilde{\Sigma}^r/\partial eV = \gamma x. \quad (23)$$

where we call  $x = \tilde{\rho}_0(0)\tilde{U} = R - 1$ , where  $R$  is the Wilson ratio mentioned in the previous section. Note that for  $\langle n_{d\sigma} \rangle = 1/2$  and  $U \rightarrow +\infty$ , corresponding to the Kondo limit,  $x = 1$  [43]. This means that in this limit, the position of the Kondo resonance at equilibrium remains at the Fermi energy [Eqs. (7), (11),  $\tilde{\Sigma}_\sigma^r(0) = 0$  and  $\partial\tilde{\Sigma}^r/\partial\mu = x$ ] if the chemical potential is shifted, as expected from the common wisdom on the Kondo resonance.

### 3.2. Spectral density and conductance

Using Eqs. (7), (10), (11), (21) and (23) one obtains up to quadratic terms in  $\omega$  and  $eV$ , calling for brevity  $c = \cos(\pi\langle n_{d\sigma} \rangle)$  and  $s = \sin(\pi\langle n_{d\sigma} \rangle)$

$$\begin{aligned} \frac{\rho(\omega)}{\rho(0)} &= 1 + A\frac{\omega}{\tilde{\Delta}} + B\frac{eV}{\tilde{\Delta}} + C\left(\frac{\omega}{\tilde{\Delta}}\right)^2 \\ &\quad + D\frac{\omega eV}{\tilde{\Delta}^2} + E\left(\frac{eV}{\tilde{\Delta}}\right)^2, \\ A &= 2sc, \quad B = -2\gamma xsc, \\ C &= s^2[4c^2 - 1 + x^2(1 - 2s^2)/2] \\ &\quad - sc\tilde{\Delta}\partial^2\text{Re}\tilde{\Sigma}^r/\partial\omega^2, \\ D &= \gamma xs^2[2 - 8xc^2 - x(1 - 2s^2)] \\ &\quad - 2sc\tilde{\Delta}\partial^2\text{Re}\tilde{\Sigma}^r/\partial\omega\partial eV, \\ E &= x^2s^2[\gamma^2(4c^2 - 1) + \delta(1 - 2s^2)/2] \\ &\quad - sc\tilde{\Delta}\partial^2\text{Re}\tilde{\Sigma}^r/\partial(eV)^2. \end{aligned} \quad (24)$$

This equation might be regarded as extension of the Friedel sum rule Eq. (10) to finite small frequency and bias voltage. The annoying terms in  $\text{Re}\tilde{\Sigma}^r$  enter only the second order terms and vanish for the symmetric Anderson model. Inserting the above result in Eq. (19) and deriving with respect to  $V$  the conductance up to terms of order  $V^2$  is obtained

$$G(V) = G(0) \left[ 1 + L \frac{eV}{\tilde{\Delta}} + M \left( \frac{eV}{\tilde{\Delta}} \right)^2 \right], \quad (25)$$

$$G(0) = 4\beta_L\beta_R s^2 \frac{2e^2}{h}, \quad (26)$$

$$L = 2sc(\alpha_L - \alpha_R - 2\gamma x), \quad (27)$$

$$M = C(\alpha_L^3 + \alpha_R^3) + 3D(\alpha_L - \alpha_R)/2 + 3E. \quad (28)$$

This is the main result of this work. Except for the second derivatives of  $\text{Re}\tilde{\Sigma}^r$ , the remaining quantities are given exactly in terms of the characteristic energy scale  $\tilde{\Delta}$ , the total occupation  $n = 2\langle n_{d\sigma} \rangle$  at the dot, the Wilson ratio  $R = x + 1$ , the ratio of the couplings to the leads  $\beta_\nu$  and the distribution of the potential decays  $\alpha_\nu$ . The energy  $\tilde{\Delta}$  can be obtained from thermodynamic quantities. For example from Eqs. (11), (12) and (14):

$$\tilde{\Delta} = \frac{2\pi k}{3\gamma_C} \sin^2(\pi n/2). \quad (29)$$

Up to second order in the interaction,  $\partial^2 \text{Re}\tilde{\Sigma}^r / \partial \omega^2$  has been calculated by Horvatić and Zlatić [20, 21]. However, for the reasons discussed above, we do not expect this (rather complicated) result to be accurate enough for strong interaction.

### 3.3. Particular cases

The total occupation of the dot  $n$  can be controlled by the gate voltage  $V_g$ . Assuming that the coupling to leads is not affected by  $V_g$ , the occupation  $n = 1$  maximizes  $G(0)$ . However, experimentally, the scaling properties of  $G(V, T)$  have been studied not only for  $V_g$  that maximizes  $G(0)$ , but for other values as well [1]. If one starts from the symmetric Anderson model, then by symmetry  $n = 1$  for  $V = 0$ ,  $c = \cos(\pi n/2)$  vanishes and with it all terms involving second derivatives of  $\text{Re}\tilde{\Sigma}^r$ . In this case, Eq. (25) simplifies to

$$\begin{aligned} G(V)/G(0) = 1 - \frac{(eV)^2}{2\tilde{\Delta}^2} [ & (2+x^2)(\alpha_L^3 + \alpha_R^3) \\ & - 3\gamma x(2+x)(\alpha_L - \alpha_R) \\ & + 9x^2(\gamma^2 + \beta_L\beta_R)], \end{aligned} \quad (30)$$

which is equivalent to the result found previously by Sela and Malecki using a different approach [4].

To model the voltage drops, in some works [3, 25] it has been assumed that the shift in the average chemical potential with applied voltage  $\Delta\mu = \gamma eV = 0$  [see Eq. (21)]. However, even in cases with very asymmetric couplings, the observed structure of the diamonds in  $G(V)$  indicates that  $\alpha_L \simeq \alpha_R$  [61, 62]. Taking  $\alpha_L = \alpha_R$ , then  $\gamma = (\beta_L - \beta_R)/2$ , and the coefficients of Eq. (25) simplify to

$$\begin{aligned}
L &= -2sc(\beta_L - \beta_R)x, \\
M &= s^2[c^2 - \frac{1}{4} + x^2(\frac{11}{4} - 4s^2 - 6\beta_L\beta_Rc^2)] \\
&\quad - sc\tilde{\Delta}[\partial^2 \text{Re}\tilde{\Sigma}^r / \partial\omega^2 + 3\partial^2 \text{Re}\tilde{\Sigma}^r / \partial(eV)^2].
\end{aligned} \tag{31}$$

Note that in a  $1/N$  expansion of the infinite  $U$  Anderson model, the value  $L = -2(\beta_L - \beta_R)$  has been found [24].

### 3.4. The maximum of $G(V)$

In the general case for which the linear term in  $V$ ,  $M \neq 0$ , the maximum of  $G(V)$  does not lie at  $V = 0$ , but at  $V_{\max} = -L/(2M)$ , with  $G_{\max}/G(0) = 1 - L^2/(4M)$ . We discuss the case  $\alpha_L = \alpha_R$  and  $2/3 < n < 4/3$  for which the curvature of the unperturbed quasiparticle density of states is positive [see Eqs. (11) and (14)]. In this case, because  $L \sim x$ , and  $M < 0$ , the largest possible  $G_{\max}$  is obtained for high interaction  $x = \tilde{\rho}_0(0)\tilde{U}$ . To estimate an upper bound for  $G_{\max}$ , we neglect the second derivatives of  $\text{Re}\tilde{\Sigma}^r$  in Eqs. (31) and take the maximum possible value of  $\tilde{U}/\pi\tilde{\Delta}$ , namely one, which implies  $x = s^2$  [see Eqs. (11) and (14)]. This gives

$$G_{\max} \leq 4Ps^2 \frac{2e^2}{h} \left[ 1 + \frac{4c^2(1 - 4P)}{16s^4 - 7s^2 - 3 + 24Ps^2c^2} \right]. \tag{32}$$

where the product  $P = \beta_L\beta_R$ . This function always increases with increasing  $P$ . Since the maximum value of  $P$  is  $1/4$ , one has more simply

$$G_{\max} \leq \frac{2e^2}{h} \sin^2(\pi n/2), \tag{33}$$

for  $\alpha_L = \alpha_R$  and  $|n - 1| < 1/3$ .

### 3.5. Effect of temperature

For  $n = 1$ , the effects of temperature  $T$  and voltage  $V$  on the spectral density and the conductance are additive up to total second order in  $\omega$ ,  $T$ , and  $V$ . The corrections to the self energy and conductance for  $V = 0$  in this case, were discussed previously [3, 4, 22, 23]. In particular

$$\frac{\rho(\omega, T)}{\rho(0, 0)} = 1 - \frac{(2 + x^2)\omega^2 + (\pi x k T)^2}{2\tilde{\Delta}^2}, \tag{34}$$

$$\frac{G(T)}{G(0)} = 1 - \frac{(\pi k T)^2}{3\tilde{\Delta}^2}(1 + 2x^2). \tag{35}$$

For  $n \neq 1$ , the corrections to the self energy in second order in  $\tilde{U}$  and up to second order in  $\omega$  and  $T$  were calculated by Horvatić and Zlatić [20, 21]. There is however in general (for  $V \neq 0$ ) a term linear in  $T$  which comes from the term of order  $\tilde{U}$  in the

self energy [see Eq. (5)], or  $\partial \text{Re} \tilde{\Sigma}^r / \partial T = \tilde{U} \partial \langle n_{d\sigma} \rangle / \partial T$ . An accurate determination of the last derivative is not possible with the knowledge of the Green functions only for frequencies near the Fermi energy. For  $V = 0$ ,  $\partial \langle n_{d\sigma} \rangle / \partial T = 0$  because the system is a Fermi liquid and the lowest order correction to the occupancy goes as  $T^2$  [44].

Including only terms linear in  $\omega$ ,  $V$  and  $T$ , and using the results of the previous section one obtains

$$\frac{\rho(\omega)}{\rho(0)} = 1 + \frac{\sin(\pi n)}{\tilde{\Delta}} [\omega - \gamma x eV - \frac{zU}{2} \frac{\partial n^2}{\partial V \partial T} VT], \quad (36)$$

$$\begin{aligned} \frac{G(T)}{G(0)} = 1 + \frac{\sin(\pi n)}{\tilde{\Delta}} [eV(\alpha_L - \alpha_R - 2\gamma x) \\ - ezU \frac{\partial n^2}{\partial V \partial T} VT], \end{aligned} \quad (37)$$

where the derivative is evaluated at  $V = T = 0$ .

#### 4. Summary and discussion

Using Fermi liquid properties and non equilibrium renormalized perturbation theory, we have calculated the self energies and spectral density near the Fermi energy, and the conductance for small bias voltage  $V$  compared to the characteristic energy scale  $\tilde{\Delta}$ . We have determined exactly the linear term in  $V$  in the conductance  $G$ , in terms of the  $\tilde{\Delta}$ , the occupation of the dot  $n$  and the Wilson ratio  $R = x + 1$ . This term is different from zero if  $n \neq 1$  and if in addition either the voltage drop is asymmetric ( $\alpha_L \neq \alpha_R$ ) or the coupling to the leads is asymmetric ( $\beta_L \neq \beta_R$ ). It is important to interpret experiments, because due to the measurement method, there is a small voltage offset [61]. For  $\alpha_L = \alpha_R$ , the sign of this term and its dependence on  $\beta_L - \beta_R$  agrees with previous results based on a  $1/N$  expansion of the infinite  $U$  Anderson model [24]. In addition, the observed  $G(V)$  is asymmetric with a  $V^3$  term [61], which is unfortunately beyond the validity of our approach, because the current is conserved only to order  $V^3$ .

For an accurate calculation of the terms quadratic in  $V$  when  $n \neq 1$ , it is necessary to know second derivatives of the real part of the self energy with respect to  $V$  and frequency  $\omega$ . These might be calculated combining numerical-renormalization-group (NRG) calculations [53] with renormalized perturbation theory [23, 49]. For  $n \neq 1$  and finite bias voltage  $V$ , there is a correction of the real part of the self energy with temperature  $T$ , proportional to  $\partial n / \partial T$ , which is also beyond the reach of low-energy expansions. For  $V = 0$ ,  $\partial n / \partial T = 0$  [44], but this is not necessarily the case out of equilibrium.

Values of the Wilson ratio  $R$  for the asymmetric Anderson model can be found for example in Table VIII of Ref. [51]. In the extreme Kondo limit,  $R \rightarrow 2$  ( $x \rightarrow 1$ ) and  $n \rightarrow 1$  simultaneously. Then, the effects of asymmetry and the coefficients of the second derivatives of the real part of the self energy tend to vanish.

The shape of the diamonds in experiments suggest a symmetric voltage drop ( $\alpha_L = \alpha_R$ ) [62], except in arrangements like that of a scanning tunneling microscope, for

which there is a very asymmetric coupling of the nanoscopic systems to the conductors ( $\beta_L/\beta_R \gg 1$  or  $\beta_L/\beta_R \ll 1$ ). In the latter case, the conductance is very small, due to the factor  $\beta_L\beta_R$  in the expression for the conductance [see Eq. (25) and (26)]. For  $\alpha_L = \alpha_R$  and  $|n - 1| < 1/3$ , we obtain the maximum of the conductance remains below the quantum of conductance times  $\sin^2(\pi n/2)$ , neglecting the effect of second derivatives of the real part of the self energy.

These terms disappear for  $n = 1$ . This situation can be searched experimentally adjusting the gate voltage in order to obtain the maximum equilibrium conductance ( $V \rightarrow 0$ ). In this limit, our results coincide with those obtained previously, using a different approach [4]. If in addition, the voltage drop is symmetric, the conductance up to second order in  $T$  and  $V$  has a very simple expression [63]

$$G = 4\beta_L\beta_R \frac{2e^2}{h} \left[ 1 - \frac{(\pi kT)^2}{3\tilde{\Delta}^2} (1 + 2x^2) - \frac{(eV)^2}{4\tilde{\Delta}^2} (1 + 5x^2) \right]. \quad (38)$$

The ratio of the coefficient of  $(eV)^2$  to that of  $(kT)^2$  lies between  $3/(2\pi^2) = 0.152$  in the strong coupling limit ( $x = 1$ ) to half of this value in the non-interacting case ( $x = 0$ ). Reported values are  $0.10 \pm 0.015$  (Ref. [1]),  $0.15$  [7] and  $0.051 \pm 0.01$  (Ref. [2]). The latter seems inconsistent with the predictions of the impurity Anderson model.

*Note added:* After acceptance of this work we became aware of Ref. [64], which addresses a similar problem for the particular case  $\gamma = 0$  ( $\alpha_L = \beta_R$ ) using a perturbative approach in  $\tilde{\varepsilon}_{eff}^\sigma$ . According to the results presented, this approach up to terms of total second order, leads to the same equations as in the Ng approximation [59, 60] [ $\tilde{\Sigma}^<(\omega) = 2i\tilde{f}(\omega)\text{Im}\tilde{\Sigma}^r(\omega)$ ], which trivially leads to the conservation of the current [see Eq. (22)], but is unfortunately incorrect, as discussed in Section 3.1.

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